

The superconducting state in the B₂H₆ compound at 360 GPa

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In the paper, the thermodynamic properties of the superconducting state in the B₂H₆ compound have been characterized. The pressure of 360 GPa has been taken into account. The calculations have been carried out in the framework of the Eliashberg formalism for the wide range of the Coulomb pseudopotential: $\mu^* \in \langle 0.1, 0.3 \rangle$. It has been found that the critical temperature (T_C) varies in the range from 147 K to 87 K, depending on the assumed value of the Coulomb pseudopotential. The ratio of the energy gap to the critical temperature ($R_\Delta \equiv 2\Delta(0)/k_B T_C$) significantly exceeds the value predicted by the BCS theory: $R_\Delta \in \langle 4.24, 3.98 \rangle$. In the similar manner behaves the ratio of the specific heat jump to the heat of the normal state ($R_C \equiv \Delta C(T_C)/C^N(T_C)$), namely: $R_C \in \langle 2.33, 2.17 \rangle$. The parameter $R_H \equiv T_C C^N(T_C)/H_C^2(0)$, where $H_C(0)$ is the thermodynamic critical field, ranges from 0.144 to 0.168.

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The intensive researches on the properties of the superconducting state have lasted for over a hundred years [1]. Their main goal is to get the material in which the superconducting state would exist at the room temperature. So far, the highest critical temperature (T_C) equal to 164 K has been measured in the HgBa₂Ca₂Cu₃O_{8+y} superconductor, located under the pressure at ~ 31 GPa [2]. However, due to the lack of the acceptable theory of the superconducting state in cuprates, it is difficult to answer the question whether in the present group of the materials might be possible to get even higher value of T_C [3].

In 1968, Ashcroft has suggested that the metallic hydrogen under the action of the high pressure would be the room-temperature superconductor [4]. Later, after the complicated numerical calculations, it has been found that the pressure of the metallization (p_m) for the hydrogen molecular phase equals about 400 GPa [5]. Thus, in the questioned pressure range, the existence of the superconducting state with the very high critical temperature can be expected [6], [7], [8], [9].

Increasing in the value of the pressure up to ~ 500 GPa causes the dissociation of the hydrogen into the atomic phase. It should be noted that near the pressure of the molecular dissociation ($p = 539$ GPa), the critical temperature can be equal to 360 K [10].

Currently, the highest value of T_C for the metallic hydrogen is expected for the pressure at 2 TPa. In the considered case, the critical temperature can reach up 600 K [11], [12], [13].

Due to the fact that the superconducting state in the

metallic hydrogen can be formed only for very high pressures, scientists began to look for other physical system, in which T_C takes high value, while p_m is relatively low. Based on the survey, it has been found that the most interesting group is the family of the hydrogen-rich compounds [14], [15], [16], [17], [18], [19], [20]. For example, in the silicon compounds Si₂H₆ ($p = 275$ GPa) and SiH₄(H₂)₂ ($p = 250$ GPa), the maximum of the critical temperature takes the values of 173 K and 130 K, respectively [21], [22].

In the present paper, we have described the results obtained for the superconducting state in the B₂H₆ compound ($p = 360$ GPa) [23]. Due to the high value of the electron-phonon coupling constant ($\lambda = 1.32$), the calculations have been carried out in the framework of the Eliashberg formalism [24]. It should be noted that this formalism is the natural generalization of the classical BCS theory [25].

On the imaginary axis ($i \equiv \sqrt{-1}$), the Eliashberg equations create the infinite system of the non-linear algebraic equations with the integral kernel, which allows to determine the order parameter function ($\phi_n \equiv \phi(i\omega_n)$) and the wave function renormalization factor ($Z_n \equiv Z(i\omega_n)$). The quantity ω_n denotes the n -th Matsubara frequency: $\omega_n \equiv (\pi/\beta)(2n-1)$, where $\beta \equiv (k_B T)^{-1}$ (k_B is the Boltzmann constant). The order parameter is defined by the ratio: $\Delta_n \equiv \phi_n/Z_n$.

The open form of the Eliashberg equations can be written as:

$$\phi_n = \frac{\pi}{\beta} \sum_{m=-M}^M \frac{\lambda(i\omega_n - i\omega_m) - \mu^* \theta(\omega_c - |\omega_m|)}{\sqrt{\omega_m^2 Z_m^2 + \phi_m^2}} \phi_m, \quad (1)$$

$$Z_n = 1 + \frac{1}{\omega_n} \frac{\pi}{\beta} \sum_{m=-M}^M \frac{\lambda(i\omega_n - i\omega_m)}{\sqrt{\omega_m^2 Z_m^2 + \phi_m^2}} \omega_m Z_m, \quad (2)$$

where the pairing kernel for the electron-phonon interac-

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tion is given by the formula:

$$\lambda(z) \equiv 2 \int_0^{\Omega_{\max}} d\Omega \frac{\Omega}{\Omega^2 - z^2} \alpha^2 F(\Omega). \quad (3)$$

The spectral function ($\alpha^2 F(\Omega)$) for the B_2H_6 compound under the pressure at 360 GPa has been calculated in the paper [23]. The maximum phonon frequency is equal to 368.5 meV.

The parameter μ^* is called the Coulomb pseudopotential and serves for the modeling of the depairing Coulomb correlations [26]; θ denotes the Heaviside unit function, and ω_c is the cut-off frequency; $\omega_c = 3\Omega_{\max}$.

When carrying out the numerical calculations the finite number of the equations should be taken into account. It turns out that above simplification does not make the significant error to the final result, if the value of the considered temperature is not too low. In the study, we

have adopted $M = 1100$ and $T \in \langle T_0 = 25K, T_C \rangle$, which ensured the convergence of the functions ϕ_n and Z_n .

It is worth noting that the Eliashberg equations have been solved using the numerical procedures, which have been tested and discussed in the papers [27] and [28].

From the physical point of view, the Eliashberg equations on the imaginary axis allow to determine the critical temperature, the free energy, the thermodynamic critical field, and the specific heat of the superconducting state. However, with their help it is impossible to accurately calculate the physical value of the energy gap (2Δ) and the electron effective mass (m_e^*). To estimate the parameters 2Δ and m_e^* , the solutions of the Eliashberg equations should be analytically continued from the imaginary axis to the real axis (ω). Such is the purpose of the Eliashberg equations in the mixed representation [29]:

$$\begin{aligned} \phi(\omega + i\delta) = & \frac{\pi}{\beta} \sum_{m=-M}^M [\lambda(\omega - i\omega_m) - \mu^* \theta(\omega_c - |\omega_m|)] \frac{\phi_m}{\sqrt{\omega_m^2 Z_m^2 + \phi_m^2}} \\ & + i\pi \int_0^{+\infty} d\omega' \alpha^2 F(\omega') \left[[N(\omega') + f(\omega' - \omega)] \frac{\phi(\omega - \omega' + i\delta)}{\sqrt{(\omega - \omega')^2 Z^2(\omega - \omega' + i\delta) - \phi^2(\omega - \omega' + i\delta)}} \right] \\ & + i\pi \int_0^{+\infty} d\omega' \alpha^2 F(\omega') \left[[N(\omega') + f(\omega' + \omega)] \frac{\phi(\omega + \omega' + i\delta)}{\sqrt{(\omega + \omega')^2 Z^2(\omega + \omega' + i\delta) - \phi^2(\omega + \omega' + i\delta)}} \right], \end{aligned} \quad (4)$$

and

$$\begin{aligned} Z(\omega + i\delta) = & 1 + \frac{i}{\omega} \frac{\pi}{\beta} \sum_{m=-M}^M \lambda(\omega - i\omega_m) \frac{\omega_m Z_m}{\sqrt{\omega_m^2 Z_m^2 + \phi_m^2}} \\ & + \frac{i\pi}{\omega} \int_0^{+\infty} d\omega' \alpha^2 F(\omega') \left[[N(\omega') + f(\omega' - \omega)] \frac{(\omega - \omega') Z(\omega - \omega' + i\delta)}{\sqrt{(\omega - \omega')^2 Z^2(\omega - \omega' + i\delta) - \phi^2(\omega - \omega' + i\delta)}} \right] \\ & + \frac{i\pi}{\omega} \int_0^{+\infty} d\omega' \alpha^2 F(\omega') \left[[N(\omega') + f(\omega' + \omega)] \frac{(\omega + \omega') Z(\omega + \omega' + i\delta)}{\sqrt{(\omega + \omega')^2 Z^2(\omega + \omega' + i\delta) - \phi^2(\omega + \omega' + i\delta)}} \right], \end{aligned} \quad (5)$$

where $N(\omega)$ and $f(\omega)$ denote the Bose-Einstein and Fermi-Dirac functions, respectively.

Note that the Eliashberg equations in the mixed representation have been solved using the procedures discussed and tested in the papers [30] and [31].

In the first step, basing on the numerical analysis, the possible range of the critical temperature has been determined. It has been found that T_C varies in the range from 147 K to 87 K for $\mu^* \in \langle 0.1, 0.3 \rangle$. Thus, regardless of the physical value of the parameter μ^* , in the B_2H_6

compound, the occurrence of the high temperature superconducting state is highly expected.

It is worth noting that the value of the critical temperature can be determined by the McMillan or Allen-Dynes formula [32], [33]. However, the obtained results are significantly depressed in comparison to the results obtained directly from the Eliashberg equations.

The forms of the order parameter and the wave function renormalization factor on the imaginary axis have been presented in Fig. 1. Basing on the obtained re-

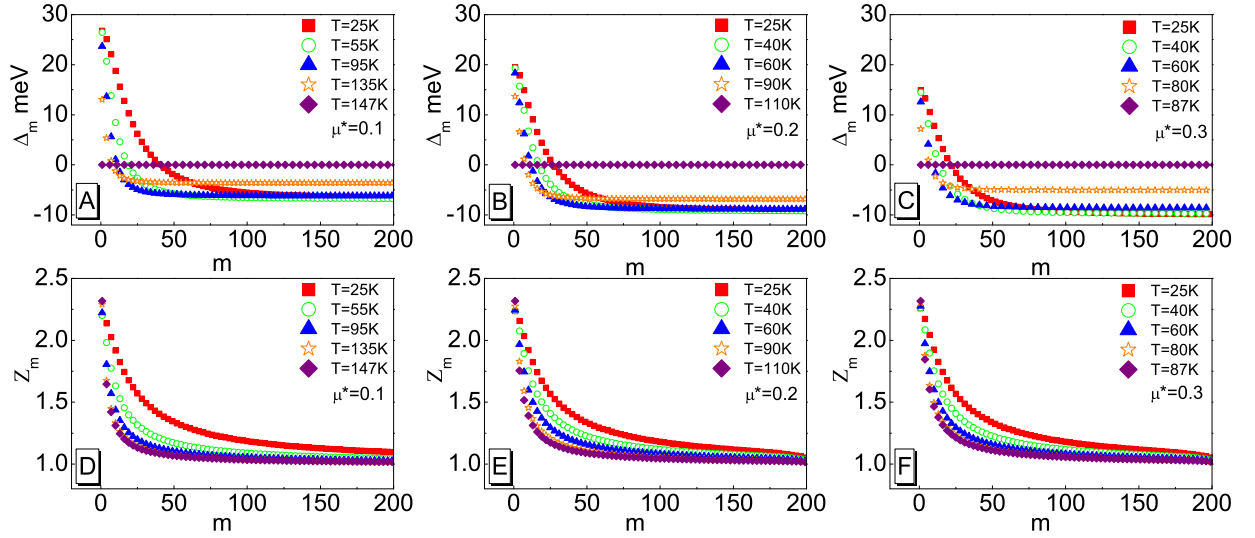


FIG. 1: (A)-(C) The order parameter and (D)-(F) the wave function renormalization factor for the selected values of the temperature and the Coulomb pseudopotential. The first 200 values of Δ_m and Z_m have been presented.

sults, it has been found that the order parameter values strongly decrease with the increasing temperature and the Coulomb pseudopotential. In turn, the wave function renormalization factor is much less dependent on T and μ^* .

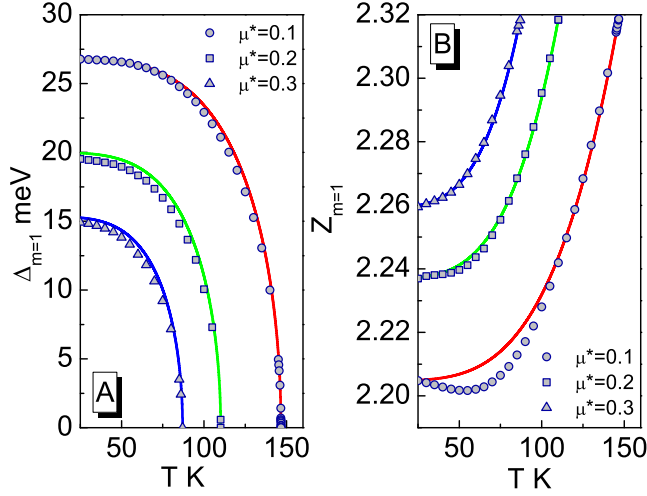


FIG. 2: (A) The order parameter $\Delta_{m=1}$ and (B) the renormalization factor $Z_{m=1}$ as a function of the temperature for selected values of the Coulomb pseudopotential. The symbols represent the exact numerical results. The solid lines have been plotted on the basis of the formulas (6) and (7).

The complete dependence of the order parameter and the renormalization factor on the temperature and the Coulomb pseudopotential can be most conveniently traced after plotting the functions $\Delta_{m=1}(T, \mu^*)$ and $Z_{m=1}(T, \mu^*)$. The obtained results have been shown in Fig. 2.

It should be noted that from the physical point of

view, the quantity $2\Delta_{m=1}(T, \mu^*)$ approximately determines the value of the energy gap at the Fermi level. On the other hand, the function $Z_{m=1}(T, \mu^*)$ is related to the effective mass of the electron. In particular: $m_e^* \simeq Z_{m=1}(T, \mu^*) m_e$, where the symbol m_e represents the electron band mass.

Let us note that the numerical results presented in Fig. 2 can be parametrized by the means of the following formulas:

$$\Delta_{m=1}(T, \mu^*) = \Delta_{m=1}(\mu^*) \sqrt{1 - \left(\frac{T}{T_C}\right)^\Gamma}, \quad (6)$$

and

$$Z_{m=1}(T, \mu^*) = Z_{m=1}(\mu^*) + [Z_{m=1}(T_C) - Z_{m=1}(\mu^*)] \left(\frac{T}{T_C}\right)^\Gamma, \quad (7)$$

where $\Gamma = 3.75$. The functions $\Delta_{m=1}(\mu^*)$ and $Z_{m=1}(\mu^*)$ can be written as:

$$\Delta_{m=1}(\mu^*) = 108.6(\mu^*)^2 - 100.9\mu^* + 35.8, \quad (8)$$

and

$$Z_{m=1}(\mu^*) = -0.484(\mu^*)^2 + 0.467\mu^* + 2.163. \quad (9)$$

The value $Z_{m=1}(T_C)$ need to be calculated on the basis of the expression: $Z_{m=1}(T_C) = 1 + \lambda = 2.32$, where $\lambda \equiv 2 \int_0^{\Omega_{\max}} \alpha^2(\Omega) F(\Omega) / \Omega$.

On the basis of the solutions of the Eliashberg equations, the free energy difference between the supercon-

ducting and normal state has been calculated [34]:

$$\frac{\Delta F}{\rho(0)} = -\frac{2\pi}{\beta} \sum_{n=1}^M \left(\sqrt{\omega_n^2 + \Delta_n^2} - |\omega_n| \right) \quad (10)$$

$$\times \left(Z_n^S - Z_n^N \frac{|\omega_n|}{\sqrt{\omega_n^2 + \Delta_n^2}} \right).$$

The symbol $\rho(0)$ denotes the value of the electron density of states at the Fermi level; Z_n^S and Z_n^N are the wave function renormalization factors for the superconducting (S) and the normal state (N), respectively.

The obtained results have been shown in the lower panels in Fig. 3. It is easy to note that the increase of the Coulomb pseudopotential results in the strong decrease of the free energy value. In particular: $[\Delta F(T_0)]_{\mu^*=0.3} / [\Delta F(T_0)]_{\mu^*=0.1} = 0.30$.

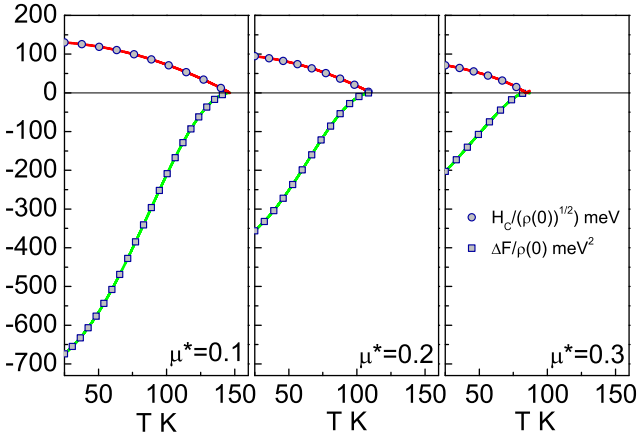


FIG. 3: (Lower panels) The dependence of the free energy on the temperature for the selected values of the Coulomb pseudopotential. (Upper panels) The thermodynamic critical field as a function of the temperature.

In the next step, the thermodynamic critical field has been determined:

$$\frac{H_C}{\sqrt{\rho(0)}} = \sqrt{-8\pi [\Delta F/\rho(0)]}. \quad (11)$$

The results have been shown in the upper panels in Fig. 3. The destructive impact of the Coulomb pseudopotential on the value of the thermodynamic critical field has been determined as: $[H_C(0)]_{\mu^*=0.3} / [H_C(0)]_{\mu^*=0.1} = 0.55$, where $H_C(0) \equiv H_C(T_0)$.

The specific heat of the superconducting state (C^S) has been calculated on the basis of the formula:

$$C^S = C^N + \Delta C, \quad (12)$$

where the specific heat for the normal state (C^N) is the linear function of the temperature: $\frac{C^N(T)}{k_B \rho(0)} = \frac{\gamma}{\beta}$. The Sommerfeld constant is equal to: $\gamma \equiv \frac{2}{3}\pi^2(1 + \lambda)$. The

difference in the specific heat between the superconducting and normal state has been determined using the formula:

$$\frac{\Delta C(T)}{k_B \rho(0)} = -\frac{1}{\beta} \frac{d^2 [\Delta F/\rho(0)]}{d(k_B T)^2}. \quad (13)$$

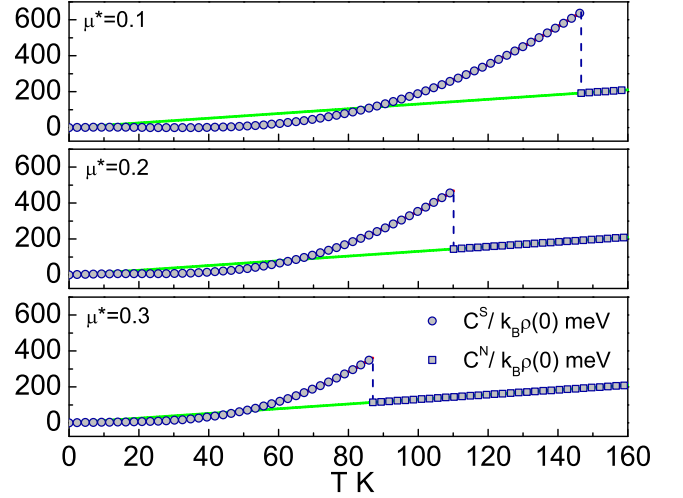


FIG. 4: The specific heat of the superconducting state and the normal state as a function of the temperature for the selected values of the Coulomb pseudopotential.

Fig. 4 presents the dependence of specific heats on the temperature and the Coulomb pseudopotential. It can be seen that at the critical temperature exists a characteristic jump, which is marked by the vertical dashed line. In addition, it should be also noted that the value of the specific heat jump strongly decreases with the increasing of Coulomb pseudopotential. In particular, the ratio $[\Delta C(T_C)]_{\mu^*=0.3} / [\Delta C(T_C)]_{\mu^*=0.1}$ equals 0.55.

Basing on the obtained results, the values of the two characteristic dimensionless ratios have been calculated:

$$R_H \equiv \frac{T_C C^N(T_C)}{H_C^2(0)}, \quad \text{and} \quad R_C \equiv \frac{\Delta C(T_C)}{C^N(T_C)}. \quad (14)$$

It has been found that in the range of the considered values of the Coulomb pseudopotential, the parameter R_H increases ($R_H \in (0.144, 0.168)$) with the increasing value of μ^* , whereas the parameter R_C decreases ($R_C \in (2.33, 2.17)$). It should be boldly underlined that in the framework of the BCS theory, the ratios R_H and R_C are the universal constants: $[R_H]_{\text{BCS}} = 0.168$ and $[R_C]_{\text{BCS}} = 1.43$ [25]. The difference between the Eliashberg predictions and the BCS theory results from the existence of the strong-coupling and retardation effects, which appear in the B_2H_6 compound.

By using the functions ϕ_n and Z_n , one can solve the Eliashberg equations in the mixed representation. The obtained results for the order parameter have been shown in Fig. 5.

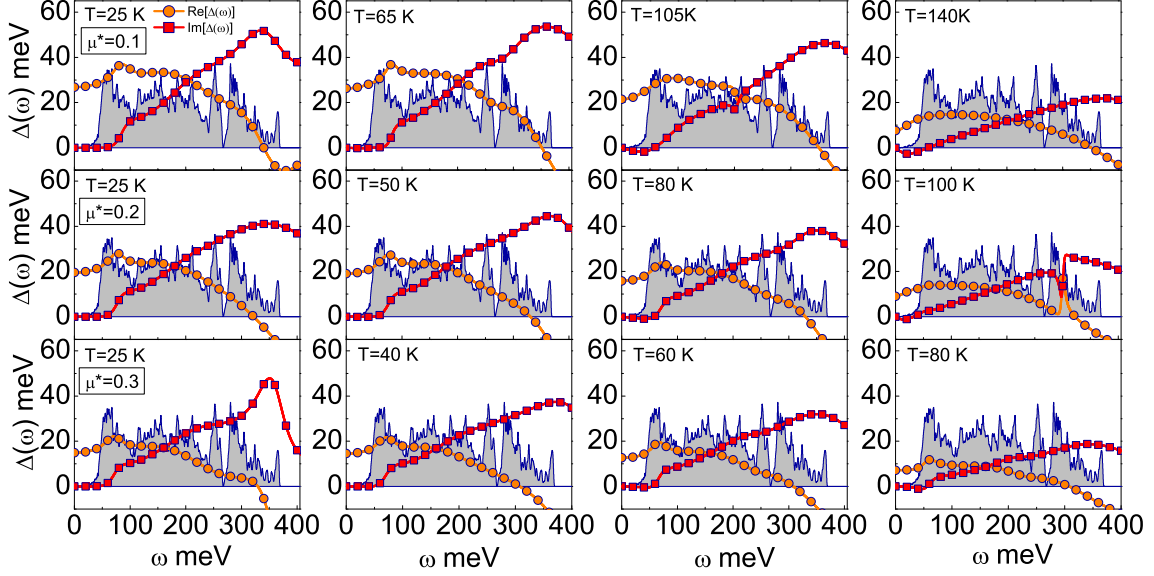


FIG. 5: The order parameter on the real axis for the selected values of the temperature and the Coulomb pseudopotential. Additionally, the rescaled Eliashberg function has been plotted ($70\alpha^2 F(\Omega)$).

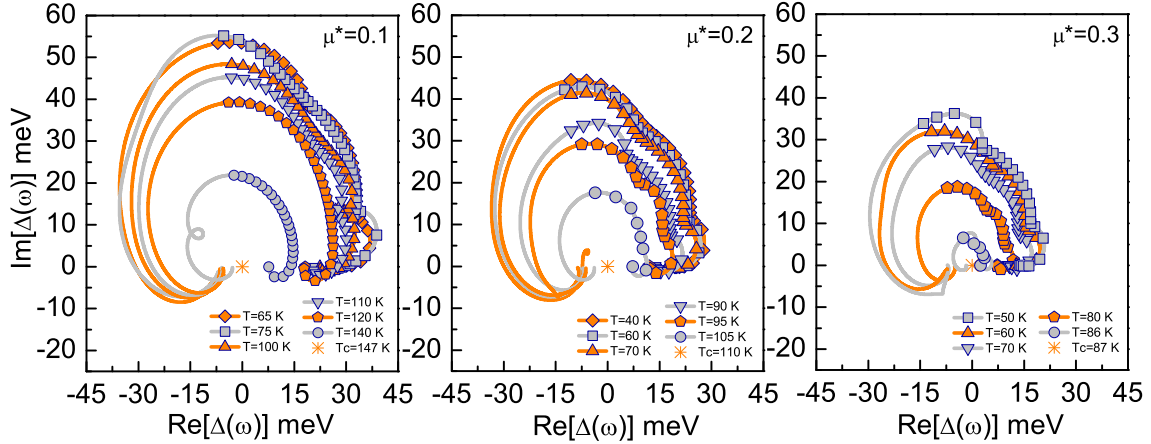


FIG. 6: The order parameter on the complex plane for the selected values of the temperature and the Coulomb pseudopotential. The lines with the symbols have been obtained for $\omega \in (0, \Omega_{\max})$; the lines without the symbols correspond to the range of the frequencies from Ω_{\max} to ω_c .

It has been found that for the low frequencies the non-zero value takes only the real part of the function $\Delta(\omega)$. This result indicates no damping effects [35]. Let us note that the imaginary part of the order parameter becomes non-zero only for the higher frequencies.

In addition, it can be easily seen that the functions $\text{Re}[\Delta(\omega)]$ and $\text{Im}[\Delta(\omega)]$ have a rather smooth course. However, the existing weak maximums or minimums are related to the corresponding peaks in the Eliashberg function.

It also seems worthy to plot the values of the order parameter on the complex plane (see Fig. 6). In the present case, the characteristic shapes of the deformed spirals can

be observed. It should be noted that the radius of the considered curves becomes strongly reduced with the increasing temperature and the Coulomb pseudopotential.

The curves presented in Fig. 6 allow in an easy way to characterize the effective potential for the electron-electron interaction. In the case when the curve meets the condition $\text{Re}[\omega] > 0$, the potential is pairing [35]. Thus, on the basis of Fig. 6, it has been found that the effective interaction between electrons leads to the formation of the superconducting condensate in the frequencies range from 0 to $\sim 0.90\Omega_{\max}$, if $\mu^* = 0.1$. The increase in the value of the Coulomb pseudopotential causes the narrowing of the considered range of ω from the side of the

higher frequencies.

The energy gap at the Fermi level has been determined on the basis of the equation:

$$\Delta(T) = \text{Re}[\Delta(\omega = \Delta(T))]. \quad (15)$$

From the physical point of view, the most interesting is the value for the lowest temperature: $2\Delta(0)$, where $\Delta(0) \equiv \Delta(T_0)$. As a result of the calculations the following has been obtained: $2\Delta(0) \in \langle 26.77, 14.91 \rangle$ meV for $\mu^* \in \langle 0.1, 0.3 \rangle$.

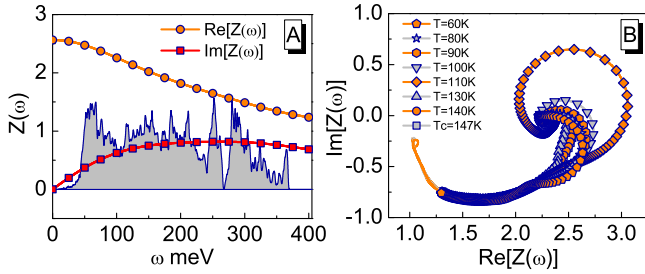


FIG. 7: (A) The wave function renormalization factor on the real axis. Additionally, the rescaled Eliashberg function has been plotted ($3\alpha^2 F(\Omega)$). (B) The wave function renormalization factor on the complex plane. The lines with the symbols have been obtained for $\omega \in \langle 0, \Omega_{\max} \rangle$; the lines without the symbols correspond to the range of the frequencies from Ω_{\max} to ω_c .

On the basis of the results above, it is very easy to estimate the value of the dimensionless parameter:

$$R_{\Delta} \equiv \frac{2\Delta(0)}{k_B T_C}. \quad (16)$$

The obtained result has the form: $R_{\Delta} \in \langle 4.24, 3.98 \rangle$. It should be noted that in the framework of the BCS theory the ratio R_{Δ} is the universal constant and it is equal to 3.53 [25]. Hence, it can be easily noticed that the BCS model is too simple to predict in the correct way the physical value of R_{Δ} for the B_2H_6 compound under the pressure at 360 GPa.

The wave function renormalization factor on the real axis for $T = T_C$ and $\mu^* = 0.1$ has been shown in Fig. 7 (A). Next, we have presented the courses of the renormalization factor on the complex plane for the selected values of the temperature.

The second solution of the Eliashberg equations allowed us to calculate the exact value of the electron effective mass: $m_e^* = Z(\omega = 0) m_e$. As a result, it has been found that in the entire temperature range, from T_0 to T_C the electron effective mass is large and it reaches its maximum value at the critical temperature ($[m_e]_{\max} = 2.56$).

In summary, in the paper we have determined all relevant thermodynamic parameters of the superconducting state in the B_2H_6 compound. The pressure of 360 GPa has been taken into account.

It has been found that, regardless assumed value of the Coulomb pseudopotential, the critical temperature is high. In particular: $T_C \in \langle 147, 87 \rangle$ K, for μ^* changing in the range from 0.1 to 0.3.

Other thermodynamic parameters differ significantly from the predictions of the classical BCS theory. This is especially visible for the low values of the Coulomb pseudopotential. In particular, it has been proven that the dimensionless ratios, characterizing the derogation from the results of the BCS theory, take the values: $R_{\Delta} \in \langle 4.24, 3.98 \rangle$, $R_C \in \langle 2.33, 2.17 \rangle$, and $R_H \in \langle 0.144, 0.168 \rangle$.

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